April 10, 2003

Sarah Loftus McLallen
Manager, CHEMSTAR
The American Chemistry Council Petroleum Additives Panel
Health, Environmental, and Regulatory Task Group (HERTG)
1300 Wilson Boulevard
Arlington, VA 22209

Dear Ms. McLallen:

The Office of Pollution Prevention and Toxics is transmitting EPA's comments on the robust summaries and test plan for Succinimide Dispersants posted on the ChemRTK HPV Challenge Program Web site on December 12, 2002. I commend The American Chemistry Council's Petroleum Additives Panel Health, Environmental, and Regulatory Task Group (HERTG) for their commitment to the HPV Challenge Program.

EPA reviews test plans and robust summaries to determine whether the reported data and test plans will provide the data necessary to adequately characterize each SIDS endpoint. On its Challenge Web site, EPA has provided guidance for determining the adequacy of data and preparing test plans used to prioritize chemicals for further work.

EPA will post this letter and the enclosed comments on the HPV Challenge Web site within the next few days. As noted in the comments, we ask that The American Chemistry Council Petroleum Additives Panel Health, Environmental, and Regulatory Task Group (HERTG) advise the Agency, within 90 days of this posting on the Web site, of any modifications to its submission.

If you have any questions about this response, please contact Richard Hefter, Chief of the HPV Chemicals Branch, at 202-564-7649. Submit questions about the HPV Challenge Program through the "Contact Us" link on the HPV Challenge Program Web site pages or through the TSCA Assistance Information Service (TSCA Hotline) at (202) 554-1404. The TSCA Hotline can also be reached by e-mail at tsca-hotline@epa.gov.

I thank you for your submission and look forward to your continued participation in the HPV Challenge Program.

Sincerely,

-S-

Oscar Hernandez, Director
Risk Assessment Division

Enclosure

cc: C. Auer
A. Abramson
W. Penberthy
M. E. Weber

EPA Comments on Chemical RTK HPV Challenge Submission:
Succinimide Dispersants

Summary of EPA Comments

The sponsor, the Petroleum Additives Panel Health, Environmental, and Regulatory Task Group (HERTG) of the American Chemistry Council, submitted a test plan and robust summaries to EPA for succinimide dispersants dated October 9, 2002. EPA posted the submission on the ChemRTK HPV Challenge Web site on December 12, 2002. HERTG subsequently submitted revised robust summaries dated December 18, 2002. EPA posted the revised summaries on the Web site on January 17, 2003.

EPA has reviewed this submission and has reached the following conclusions:

1. Category Justification. The justification provided was sufficient to support the proposed category.

2. Physicochemical Properties. EPA agrees with the test plan for these endpoints, with the possible exception of melting point. However, the rationale for no further testing needs modification.

3. Environmental Fate. EPA agrees with the test plan for these endpoints.

4. Health Effects. Adequate data are available for these endpoints for the purposes of the HPV Challenge Program. The submitter needs to address deficiencies in the robust summaries.

5. Ecological Effects. The data submitted for fish, aquatic invertebrates and algae are inadequate.

EPA requests that the submitter advise the Agency of any modifications to its submission within 90 days.

EPA Comments on the Succinimide Dispersants Challenge Submission

Category Definition

The submitter proposed a category of two sponsored succinimide dispersants: 1-[2-[[2-[[2-[(2-aminoethyl)-amino]ethyl]amino]ethyl]amino]ethyl]-2,5-pyrrolidinedione, monopolyisobutenyl derivatives (CAS No. 67762-72-5) and polyethylenepolyamines, reaction products with succinic anhydride polyisobutenyl derivatives (CAS No. 84605-20-9). The simplified names that refer to these substances in the test plan are mono alkenyl succinimide derivative and bis alkenyl succinimide derivative, respectively.

The mono alkenyl succinimide is a high molecular weight compound containing a polyisobutylene group (MW = 950-2500) bonded to 1-polyethylenepolyaminesuccinimide ([2-[[2-[[2-[(2-aminoethyl)amino]ethyl]-amino]ethyl]amino]ethyl]-2,5-pyrrolidinedione) on the ring 3-position.

The bis alkenyl succinimide derivative differs structurally from the mono alkenyl succinimide derivative by the varying size of the polyethylenepolyamine group (ranging from two to ten ethyleneamine units) and by the possible inclusion of a 3-polyisobutylenesuccinimide function at the terminal end of the polyethylene-polyamine group. The succinimide dispersants are synthesized in a “highly refined lubricating base oil” solvent and are never isolated; the commercial forms contain 25-35 wt% of the oil.

The submitter does not provide a uniform characterization of the mono or bis alkenyl succinimide derivatives. Differing ranges for the molecular weights of the polyisobutylene group are given throughout the test plan (500-2500, 250-2500, 950-2500). The submitter needs to identify the typical structure ranges and discuss the extent to which lower molecular weight species are present.

The category definition is adequate.

Category Justification

The submitter bases the category on their structural similarity and their expected similarities in physicochemical, environmental fate, and toxicological properties. Both derivatives have molecular weights above 700, and are expected to have high boiling points, low vapor pressures and water solubilities, and high partition coefficients.

No information about the characteristics of the lubricating base oil is provided in the test plan. While the physicochemical properties of the hydrocarbons in the oil likely have a significant influence on the measured physicochemical and environmental properties presented in the test plan, the succinimide molecules decomposed when the submitter attempted to deoil the mixtures, precluding measurements on the pure succinimide mixtures. Because of the difficulty in isolating the succinimide mixtures, the submitter provided estimated physical properties of "representative" structures of the chemicals in the test plan (Appendix I, Table 2). These values, though showing significant differences between the two members of the category, indicate that the two members will behave similarly in the environment. In addition, measured aquatic and mammalian toxicities for the commercial products support the similarities of these substances, and justifies extrapolation from available data on the bis derivative to address data gaps on the mono derivative.

Test Plan

Physicochemical Properties (melting point, boiling point, vapor pressure, partition coefficient, and water solubility).

EPA agrees with the submitter that adequate data are available and no additional testing is necessary for boiling point, vapor pressure, water solubility, and octanol/water endpoints. However, the proposed test matrix on page 23 of the test plan shows "C" for the physicochemical properties, which indicates computer estimation of these endpoints. Estimation is generally not appropriate for the physicochemical SIDS endpoints of polymers and so the rationale in the test plan for no further testing needs to be modified.

Melting Point. The submitter states that "succinimide derivatives, as highly refined lubricating base oils, are liquids at ambient temperature." According to OECD TG 102, melting points need to be measured for compounds that melt above 0 °C. However, the submitter should clarify what temperature the phrase "ambient temperature" refers to, and needs to test for melting point if the "oiled" succinimide derivatives melt above 0 °C.

Environmental Fate (photodegradation, stability in water, biodegradation, fugacity).

EPA agrees with the submitter's approach for photodegradation, biodegradation, and fugacity.

Photodegradation. The submitter should clarify whether succinimide dispersants are expected to absorb greater than 290 nm and undergo direct photolysis.

Stability in Water. For stability in water, the submitter proposes that a technical discussion will be provided for this endpoint. Since succinimide dispersants contain amide functional groups, which are susceptible to hydrolysis, EPA reserves judgement until the detailed discussion is available.

Fugacity. EPA agrees with the submitter's test plan for estimation based on comparison of the submitter's Level I fugacity calculations with the Level III calculations of the Agency using EPIWIN. This should be included in the robust summary for this endpoint.

Health Effects (acute toxicity, repeated-dose toxicity, genetic toxicity, and reproductive/developmental toxicity).

EPA agrees that adequate data are available for these endpoints for purposes of the Challenge program. The submitter needs to address deficiencies in the robust summaries.

Ecological Effects (fish, invertebrates, and algae).

The data provided for succinimide dispersants are inadequate. The tests were conducted above the water solubility limit of 0.125 mg/L in the case of CAS No. 67762-72-5. It appears that these chemicals are dispersible in water and should have been tested at their dispersibility limit. In addition, the chemicals were not buffered at pH 7 and the TOC were above the generally accepted 2.0 mg/L limit for low-solubility chemicals.

For future testing, test substances need to be characterized to the extent possible in terms of molecular weight and the number of repeating units. The test plan indicates that the polyisobutylene (PIB) group in the structures of both category members can range from 500 to 2500 in molecular weight. The submitter needs to provide the molecular weight range of the PIB group. Additionally, as indicated in Table 2 of the test plan, the bis alkenyl derivative has a dialkyl nitrogen that can appear up to 8 times in the structure (n = 1-8), and may contain a second PIB/ring moiety(n = 0-1). The submitter needs to define the average "n" number ranges for the bis alkenyl succinimide.

EPA suggests testing both chemicals in fish, aquatic invertebrates, and algae, using samples representing the probable worst case scenario, i.e., lowest-molecular-weight constituents and high ethylene amine repeating units (if commercially available), to provide optimal results. Tests should use measured concentrations at or below the chemicals' water solubility or at their dispersibility limits. Alternatively, the submitter can test the substance expected to be the most toxic on the basis of lowest molecular weight components and extrapolate the results to the other category member.

Specific Comments on the Robust Summaries

Generic comments

The submitter should consult EPA guidance documents for the preparation of robust summaries (http://www.epa.gov/opptintr/chemrtk/guidocs.htm).

Robust summaries for CAS No. 67762-72-5 listed the chemical name as "2,5-pyrrolidinedione." As this is a synonym for succinimide, a less confusing alternative (assuming that the tests were conducted on CAS No. 67762-72-5 and not on succinimide) such as "mono alkenyl succinimide derivative" is advisable.

Summaries should explicitly state if substance purity information was not reported.

Physicochemical Properties

The submitter needs to provide robust summaries explaining why measured data are unnecessary for this category (see test plan discussion above).

Vapor pressure. A robust summary needs to be provided for the study that reports low vapor pressures ($<10^{-10}$ Pa or 7.5×10^{-13} mm Hg at 25 °C) for highly refined base oils.

Partition coefficient. The submitter needs to provide a robust summary for the study that states that the partition coefficient of 6.7 was measured for a representative succinimide dispersant, mono alkenyl succinimide derivative (CAS# 67762-72-5).

Water solubility. The submitter needs to provide a robust summary and citation for the study that states that a water solubility of 0.125 mg/L was measured for a representative succinimide dispersant, mono alkenyl succinimide derivative (CAS# 67762-72-5).

Environmental Fate and Transport

The submitter needs to provide robust summaries with the proposed technical discussion of hydrolysis and fugacity modeling, including results and input parameters.

Biodegradation. If possible, the submitter should clarify whether the test compound was pure succinimide dispersant or the dispersant in 25-35% highly refined lubricating base oil.

Photodegradation. The submitter needs to provide a robust summary for the AOPWIN model results as well as input parameters. The summary should also discuss whether succinimide dispersants absorb at >290 nm.

Health Effects

Repeated-Dose Toxicity. The robust summary for a dermal toxicity study on CAS No. 67762-72-5 needs to include the doses expressed on a *weight* per kg body-weight basis.

Followup Activity

EPA requests that the submitter advise the Agency of any modifications to its submission within 90 days.